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A Comprehensive X-Ray Spectral Code for High Energy Astrophysics

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A COMPREHENSIVE X-RAY SPECTRAL CODE FOR HIGH ENERGY ASTROPHYSICS

FINAL REPORT

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ABSTRACT

The aim of this project has been to develop a spectral analysis tool with a level of quality and completeness commensurate to that expected in data from the current generation of X-ray observatories. The code is called LXSS (Livermore X-Ray Spectral Synthesizer). X-ray-emitting astrophysical plasmas are rarely, if ever, in LTE, so we have adopted the detailed level accounting approach, in which rates for processes that populate or depopulate atomic energy levels are treated explicitly. This entails the generation of a large quantity of atomic data, most of which is calculated using "in-house" computer codes. Calculations are benchmarked against laboratory data, and spectral models have been used to provide first-time interpretations of astrophysical X-ray spectra. The design of a versatile graphical user interface that allows access to and manipulation of the atomic database comprises the second major part of the project.

1. THE NEW GENERATION OF X-RAY OBSERVATORIES

The international commitment to advancing the field of X-ray astronomy is evidenced by the recent launches of NASA's *Chandra X-ray Observatory* (Aug 1999) and the European Space Agency's *X-Ray Multi-Mirror Mission* (*XMM*; Dec 1999). Unfortunately, a third major mission, *Astro-E*, a cooperative effort by Japan and the U.S., failed to achieve orbit. The simultaneous deployment of two facility-class X-ray satellites, comprising several billion dollars of space hardware, heralds a potential revolution in the field.

The mission objectives of *Chandra*, and *XMM* are predominantly spectroscopic: they carry spectrometers that, combined, cover the 1-160 Å band, with large collecting areas (hundreds of square centimeters) and high spectral resolving powers ($\lambda/\Delta\lambda$ of several hundred). These missions thus offer astronomers and astrophysicists their first opportunity to obtain high-quality X-ray spectra from extrasolar X-ray sources. With their projected ten-year lifetimes, thousands of X-ray datasets will be generated, representing almost every class of celestial object: stellar coronae, supernova remnants, normal galaxies, clusters of galaxies, white dwarfs, neutron stars, and black holes. An understanding of spectral formation leads to an understanding of the source physics.

2. ASTROPHYSICAL X-RAY LINE SPECTROSCOPY AND SPECTRAL SYNTHESIS

In terms of scientific data, the most salient aspect of *Chandra* and *XMM* is that, for the first time, X-ray *line* spectroscopy will become the central theme of X-ray astronomy. It has been remarked that we are about to see the field make a transition from astronomy to astrophysics. Facilitating this transition, however, is problematic, a lesson brought to us by the previous major X-ray mission, the *Advanced Satellite for Cosmology and Astrophysics* (*ASCA*; launched in 1993), which was a joint effort of Japan and the U.S. Even though the CCD spectrometers aboard *ASCA* lacked the high resolving powers of *Chandra* and *XMM*, it became evident that the theoretical tools available for spectroscopic analysis were not up to the task.

Theoretical models of X-ray line spectra are generated by computer codes called *spectral synthesis codes* (SSCs), which provide the means to translate observed spectra into statements of the source physics. In essence, an SSC allows access to and manipulation of one or more databases containing atomic quantities. The atomic quantities consist of energy level structure, radiative decay rates, collisional excitation rates, photoionization cross-sections, and so forth. This information is used to calculate level population distributions for each ion at a given temperature and density, from which follows the emission-line spectrum. Also calculated are the continuum radiation processes: ion-electron bremsstrahlung, two-photon decay, and radiative recombination. Detailed data for the elements hydrogen, helium, carbon, nitrogen, oxygen, neon, magnesium, silicon, sulfur, argon, calcium, and iron are mandatory in order to generate a reasonable model spectrum of a typical celestial X-ray source. Of somewhat less importance, but required to achieve completeness, are data for the elements sodium, aluminum, and nickel. For each element, every charge state with bound electrons falls within the purview of a complete SSC, giving a total of 179 ions.

Modern SSCs are not "hardwired" to use a particular set of atomic data. Rather, they access databases that are modular in design; as improved atomic data become available, the obsolete data are simply replaced, requiring no explicit modifications to the SSC. Data come to SSC developers in a variety of formats, and come from a mix of experimental and theoretical work. Considerable effort is expended in maintaining familiarity with the literature, acquiring new atomic data, and reformatting it into a form that the SSC can ingest. Thus a division of labor has evolved: data generators (maybe a hundred scientists) provide data to SSC developers (a few scientists), who facilitate access to atomic data for users (thousands of scientists). This division is not strictly adhered to, of course, but it adequately represents the "culture" of X-ray astronomy.

3. THE LXSS PROJECT

In the early 90s, coming into the field primarily as observers and modelers, we began also to play the role of generators of atomic data to several of the major SSC development groups. Slow turnaround times and quality control issues surfaced as problems, however. Moreover, although we were in the habit of regularly generating state-of-the-art atomic models, they were usually designed for a specific problem, and lacked generality. We were left with a large non-uniform, unwieldly database, unsuitable for astrophysical data analysis. These various factors led us to the conclusion that our interests could be better served by constructing our own SSC. Our team has significant overlap with all three groups delineated above: as observers/analysts, we are familiar with the desired scope and functions of SSCs; as data generators, we can assemble a highly-customized database and impose our own standards of quality; as SSC developers, we are able to design a code that facilitates our own research activities.

3.1 Construction

With LDRD funding we began work on the Livermore X-ray Spectral Synthesizer (LXSS). The tasks laid out for us were:

(1) generation of the bulk of the atomic database using LLNL computer codes
(2) compilation, critical assessment, and incorporation of atomic data that cannot be generated at LLNL in a timely manner
(3) design of a user interface that will allow rapid manipulation of the database

3.1.1 Collisionally Ionized Plasmas

A large part of the database has been generated using the HULLAC (Hebrew University/Lawrence Livermore Atomic Code) suite. HULLAC gives us the means by which to quickly generate atomic structure calculations, radiative and autoionization transition rates, and electron-ion collisional excitation rate coefficients. Along with the charge state distributions of each element at a given temperature, these constitute the essential components of an SSC designed for application to plasmas in coronal ionization equilibrium (CIE). In fact, most of the "production" codes are designed for this environment. Coronal ionization equilibrium applies to stellar coronae, clusters of galaxies, and probably interstellar media. The shocked gas in supernova remnants may be in a transient phase of ionization disequilibrium, but the level population kinetics is much the same as in CIE. LXSS includes a differential equation solver that determines the charge state distribution as a function of time under transient conditions.

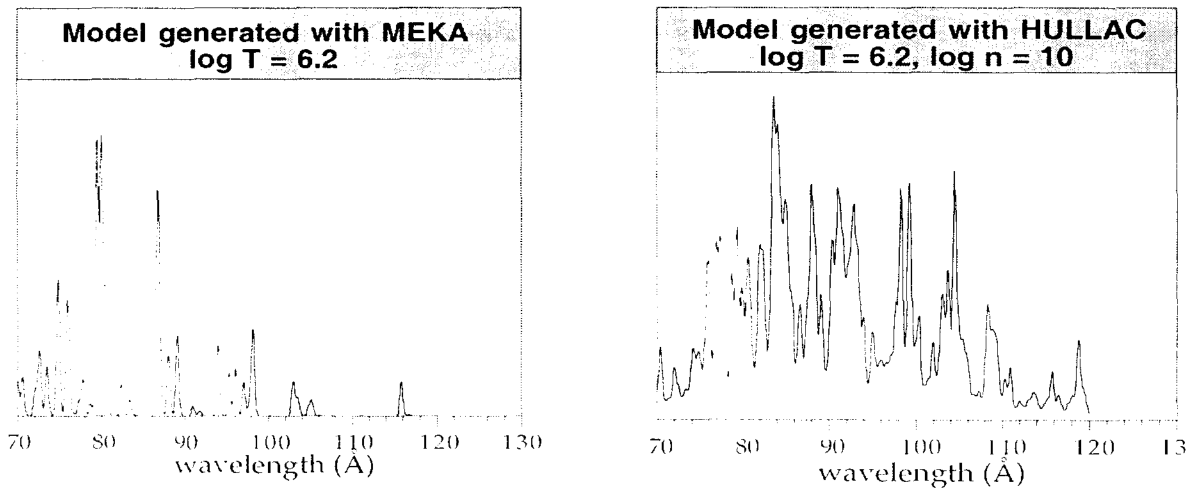

Figure 1. Comparison of model spectra predicted by two models: (*left panel*) the MEKA code, which is currently the best publicly available SSC in this spectral range and (*right panel*) LXSS. This comparison exemplifies the "missing line" problem in X-ray astronomy. The electron density for the LXSS run is chosen as characteristic of stellar coronae. Note that the MEKA model makes no provision for density dependence, since it does not invert a rate matrix for the level populations.

3.1.2 Photoionized Plasmas

The other important class of ionization dynamics is photoionization equilibrium, in which photons, rather than electrons, are primarily responsible for ionizing atoms. In photoionized gas, the charge state fraction of a given ion peaks at a temperature that is much lower than in CIE. Radiative and dielectronic recombination dominate the level population kinetics in a photoionized gas. In addition to those listed in §3.1.1, the essential atomic physics ingredients for these calculations are photoionization cross-sections, which permit the calculation of radiative recombination cross-sections from a detailed balance relationship. We have constructed atomic and spectral models appropriate for this regime, and included them in LXSS, which makes LXSS unique with respect to other SSCs. While it is true that the class of codes called photoionization codes include recombination spectral models, the LXSS models are the current state-of-the-art. Photoionization equilibrium applies to quasars, Seyfert galaxies, and X-ray binaries.

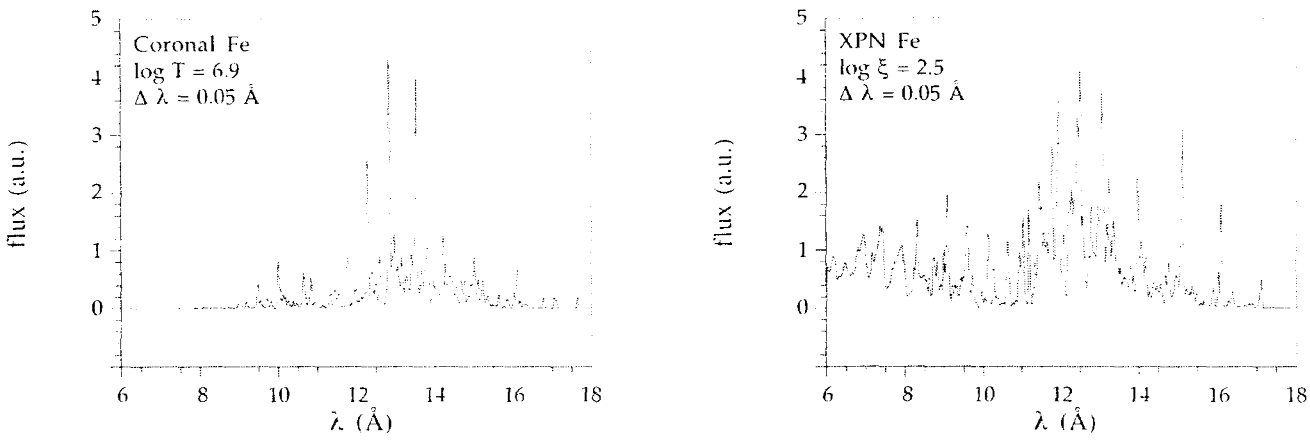

Figure 2. Comparison of LXSS iron spectra for two types of ionization equilibria: (*left panel*) collisional ionization equilibrium and (*right panel*) photoionization equilibrium. The charge state distribution in either case corresponds to conditions for which C-like Fe XXI attains its peak. The model spectrum is folded through a gaussian resolution kernel chosen to approximate the spectral resolving power of the *XMM* gratings.

3.1.3 Atomic Database

Table 1 lists some of the ingredients of LXSS, and gives an indication of the large degree to which the LXSS database is generated with LLNL resources. Atomic data are stored in a binary format known as FITS (Flexible Image Transport System) format, for easy interface with fitting packages provided by NASA centers. We have written several "pipeline processing" codes in IDL (Interactive Data Language) to facilitate uniform data conversion and storage. An extensive IDL graphical user interface, which allows access to a number of simulation and display functions, and a database query function, are now operational.

The ability to generate the vast majority of the required atomic data ourselves gives us several advantages over other SSC groups. For example, we choose the atomic model size and the physical parameter space over which it validly operates, rather than being forced to setltle for what is available in the literature. Since we can create and format atomic data much more rapidly than the community of generators, lag times are much shorter.

TABLE 1 Atomic physics and modeling options contained in LXSS classified according to origin.

Feature	*Internal Sources*	*External Sources*
atomic atructure	✓	
radiative transition rates	✓	
two-photon transition rates		✓
autoionization rates	✓	
photoionization cross-sections	✓	
electron-ion impact cross-sections	✓	
proton-ion impact cross-section		✓
collisional ionization rates		✓
dielectronic recombination rates/satellite spectra	✓	
bremsstrahlung continuum		✓
radiative recombination continuum	✓	
charge state distribution	✓	✓
jj-averaging and *n*-averaging	✓	
line and ion continuum opacity	✓	
graphical user interface	✓	

3.2 Benchmarking

Even the most sophisticated computer codes run up against limitations. In calculating atomic energy level structure, for example, an intrinsic error ΔE translates into a wavelength error $\Delta\lambda$ that scales as λ^2. In other words, wavelength predictions get rapidly worse moving from the X-ray band towards the ultraviolet band. In the ~10 Å region, HULLAC wavelengths have been shown to be accurate typically to within roughly a part in 1000, while near 100 Å (EUV) the accuracy is closer to a part in 100, which is unacceptably large for current applications. Fortunately, errors of this order are not catastrophic; code output can be adjusted "by hand" to conform to experimental data, where that data exists, and where it is reliable. We have benefitted from close collaborations with experimentalists involved with tokamaks and the Electron Beam Ion Trap (EBIT) at LLNL, as well as observers involved with orbiting observatories such as the *Extreme Ultraviolet Explorer* (*EUVE*) and *ASCA*. Data acquired with these facilities provide suitable testbeds and standards against which to evaluate and improve the quality of our calculations.

Without going into great detail, we can say the LXSS models have fared extremely well in comparisons against laboratory data. We have found cases where the omission resonant excitation in our models leads to errors in predicted intensities of order 30%, most noticably in the EUV spectral range. Shortcomings of this type are corrected most easily by supplementing HULLAC data with the results of more exact calculations (see Table 1) which use, for example, an R-matrix code. It is worth emphasizing that in the harder X-ray band (λ < 35 Å), EBIT experiments show that HULLAC (hence, LXSS) models perform at a high level of accuracy. In collaborations with groups in England, Holland, and the U.S., we are applying small wavelength corrections to our models in order to conform to the highly precise measurements obtained in tokamaks, EBIT, the solar corona, and stellar coronae which are now available.

3.3 Applications

Although LXSS has yet to be released, we are already using models that constitute its raw ingredients to analyze and interpret spectra from both celestial and terrestrial sources. An appreciation of the scope of these activities can be gained through an examination of the titles listed in Part 5. Two highlights: (1) Using high-resolution X-ray spectroscopy of neon and argon emission from a well-diagnosed magnetically confined fusion plasma, it was demonstrated that resonance enhancement of direct collision rates needs to be taken into account in simulating transitions between excited atomic states. This is crucial for correctly implementing spectroscopic diagnostics of local particle transport in tokamaks, which, in turn, is required in order to understand the overall energy balance inside the plasma. (2) In X-ray astronomy, we have obtained, for the first time, a broad band spectral fit to the discrete X-ray spectrum of a neutron star X-ray binary using a spectral model based on actual atomic physics, rather than an arbitrarily adjustable empirical model. This has allowed us to derive physical constraints of the accretion flow in the high-mass X-ray pulsar Vela X-1. Since the LXSS project was begun prior to the launches of *Chandra* and *XMM*, the primary scientific drivers for this project, the most exciting applications are yet to come.

4. OUTLOOK

The construction phase of LXSS as an astrophysics interpretive tool is near an end. While it's true that such codes can never really be finished, since new developments in atomic physics continually lead to improvements in the quality of the atomic database, we have reached our first major plateau. Our close involvements in X-ray astronomy and laboratory spectroscopy will provide a wealth of applications. We have been awarded a number of PI Guest Observerships on *Chandra*, *XMM*, and *Astro-E*, and are participants in the *XMM* Guaranteed Time program (we were extremely successful in the Cycle 1 review of the ill-fated *Astro-E*.). Over the next few years, we thus foresee many excellent opportunities to exercise the full capability of LXSS. We expect LXSS to evolve to the point where, in addition to astrophysical applications, it supports all internal X-ray spectroscopic modeling and interpretation.

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